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Original

Simulation of particle deposition in porous media: computational fluid dynamics and population balance modelling / Boccardo, Gianluca; Crevacore, Eleonora; Sethi, Rajandrea; Marchisio, Daniele. - (2015). ((Intervento presentato al convegno 10th European Congress of Chemical Engineering tenutosi a Nice (FRA) nel September 27th - October 1st 2015.

Availability:

This version is available at: 11583/2619253 since: 2015-10-06T16:53:09Z

Publisher:

Published

DOI:

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Simulation of particle deposition in porous media: computational fluid dynamics and population balance modelling

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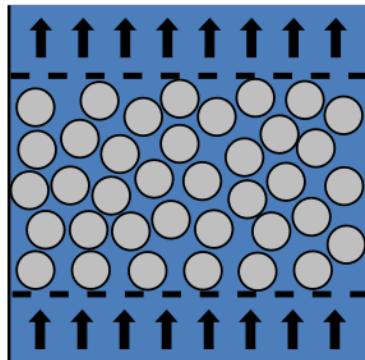
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September 29, 2015

Motivation of the work

Many fields of interest

- Packed bed reactors
- Filtration
- Chromatographic Separation
- Aquifer Remediation
- Enhanced Oil Recovery



- Fluid flowing through an arrangement of stationary solid grains.
- The flowing fluid can contain liquid droplets, gas bubbles or solid particles.

Computational models structure

POROUS MEDIUM GENERATION

- Experimental:
 - μ -CT, X-ray, SEM
- Algorithmic reconstruction:
 - DEM, particle-based
 - Rigid body simulation
 - **Blender (opensource)**

FLOW, TRANSPORT SIMULATION

- Computational Fluid Dynamics
 - Ansys FLUENT (commercial)
 - **OpenFOAM (opensource)**

⇒ Model of porous medium with **Blender**

⇒ Meshing and CFD simulation with **OpenFOAM**

Dispersion in 3D Porous Media

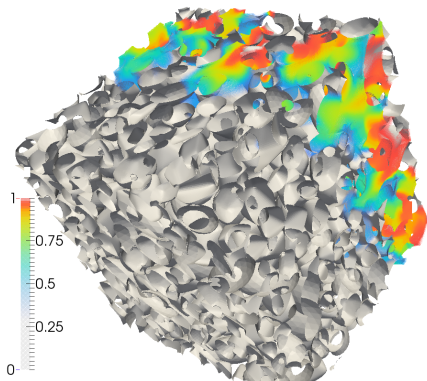
Simulation Setup

GEOMETRY

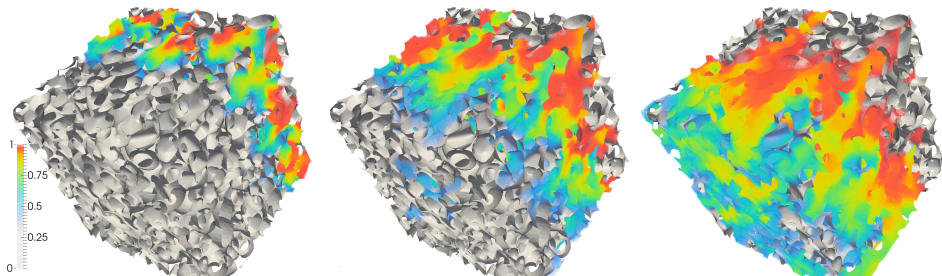
- 2mm cubic sample
- 3000 grains
- 40M cells

OPERATING CONDITIONS

- Particle diameter:
 $d_p = 1 \div 1000 \text{ nm}$
- Superficial velocity:
 $q = 10^{-6} \div 0.1 \text{ ms}^{-1}$
- $10^{-4} < \text{Re} < 300$
- $10^{-2} < \text{Pe} = \frac{qD_g}{D_m} < 10^7$



Hydrodynamic Dispersion



Snapshots of particle concentration at three different times

- Hydrodynamic dispersion enlarges and smoothens out the particle concentration front over time
- This effect increases for higher Péclet numbers

Particle Deposition

Deposition Efficiency

BROWNIAN DIFFUSION

$$\eta_B = 4.04\text{Pe}^{-\frac{2}{3}}$$

Yao-Levich

$$\eta_B = 4\text{As}^{\frac{1}{3}}\text{Pe}^{-\frac{2}{3}}$$

Happel

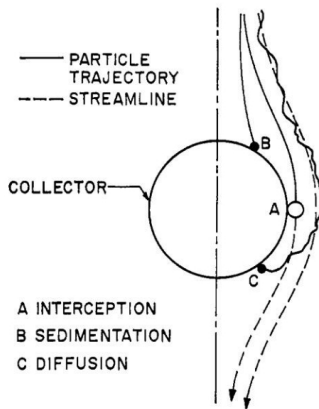
INTERCEPTION

$$\eta_I = \frac{3}{2} \left(\frac{d_p}{D_g} \right)^2 = \frac{3}{2} N_R^2$$

Yao-Levich

$$\eta_I = \frac{3}{2} \text{As} N_R^2$$

Happel



Particles Modeling

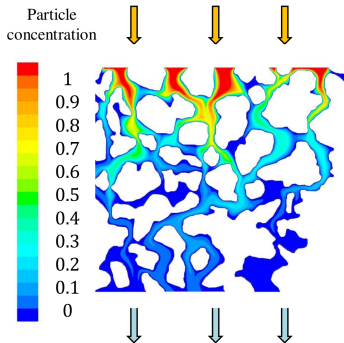
Particles are transported by convective and diffusive phenomena

BOUNDARY CONDITION

- $C = 1$ at inlet
- $C = 0$ on grain surface (assumed "perfect sink" B.C.)

OPERATING CONDITIONS

- Particle diameter:
 $d_p = 1 \div 1000 \text{ nm}$
- Superficial velocity:
 $q = 10^{-6} \div 0.01 \text{ ms}^{-1}$

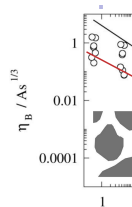
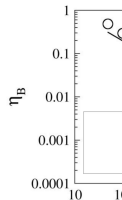
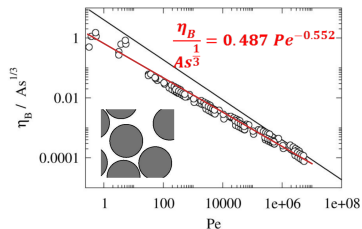
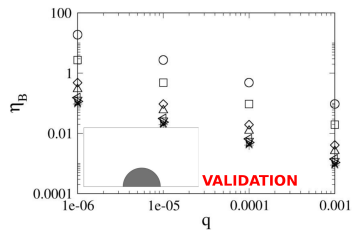


Collector deposition efficiency, η
calculated with packed bed
performance equation

$$\frac{dC}{dx} = -\frac{3}{2} \frac{1-\varepsilon}{\varepsilon D_g} \eta C$$

Results: Particle Deposition

Deposition Efficiency: Brownian Diffusion



Population Balance Modelling

Population balance equation

- evolution of the particle size distribution
- possibility of treating a polydisperse particle population

Solution of the PBE in the CFD code with the Method of Moments

$$\frac{\partial m_k}{\partial t} + \frac{\partial \mathbf{u} m_k}{\partial \mathbf{x}} = \frac{\partial}{\partial \mathbf{x}} \left(\Gamma_0 \frac{\partial m_{k-1}}{\partial \mathbf{x}} \right)$$

Deposition of polydisperse particle populations

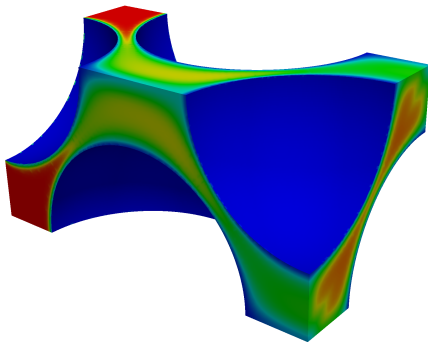
Simulation Setup

GEOMETRY

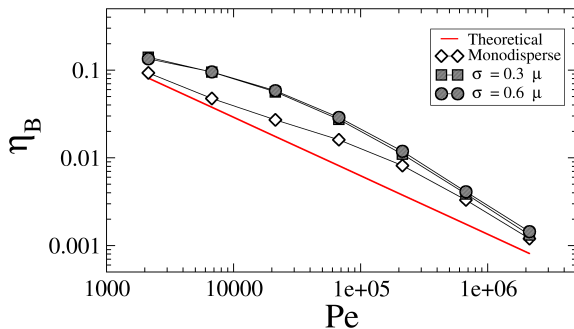
- Domain = one grain
- Face-centered cubic
- 260k cells

OPERATING CONDITIONS

- Mean particle diameter:
 $\mu = 300 \text{ nm}$
- $10^{-3} < \text{Re} < 3$
- Two lognormal distributions:
 - $\rightarrow \sigma = 0.3 \mu$
 - $\rightarrow \sigma = 0.6 \mu$

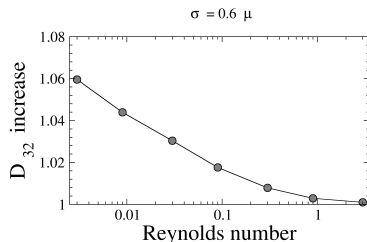
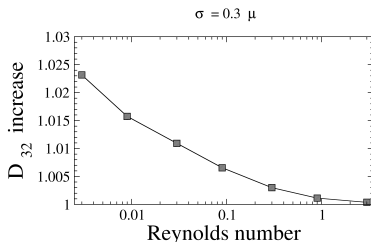


Results: Deposition rates of polydisperse particle populations



- Very different η - Pe relationship w.r.t to monodisperse case and theoretical prediction.
- Weak effect of particle population polydispersity.

Results: Increase in average diameter



- Higher σ means more deposition of smaller particles, hence an increase of average particle diameter.
- Behaviour of particle population changes in space during the evolution of the dispersion process
→ e.g. effect on reaction rates, dispersion coefficient, et c.

Conclusions

Micro-scale modeling is essential
to the derivation of effective macro-scale models

Classic deposition laws fail with:

- realistic (non-spherical) geometries
- polydisperse particle populations
- Possibility of treating packings of arbitrary grain shape with BLENDER
- Treatment of polydisperse particle populations via population balance modelling shows an improvement over theoretical predictions

Acknowledgements - People

DIATI - Politecnico di Torino (I)

- Tiziana Tosco (Ass. Prof.)
- Francesca Messina (Post-Doc. Res.)

Warwick University (UK)

- Matteo Icardi (Assistant Professor)

Acknowledgements - Resources

Financial Resources

- AQUAREHAB (FP7, Grant Agreement no. 226565)
- PRIN Project 2008:
“Disaggregazione, stabilizzazione e trasporto di ferro zerovalente nanoscopico”

Computational Resources

- PRACE Research Infrastructure
- CINECA

Thank you!